

# On entropy production for controlled Markovian evolution

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## Abstract

We consider thermodynamic systems with finitely many degrees of freedom and subject to an external control action. We derive some basic results on the dependence of the relative entropy production rate on the controlling force. Applications to macromolecular cooling and to controlling the convergence to equilibrium rate are sketched. Analogous results are derived for closed and open  $n$ -level quantum systems.

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## I. INTRODUCTION

Advances in nanotechnology permit nowadays to implement feedback control actions on nanodevices. For instance, in surface topography, the deflection of a cantilever is captured by a photodetector that records the angle of reflection from a laser beam focused on the mirrored surface on back side of the cantilever. Position feedback control is used to maintain the probe at a constant force or distance from the object surface. Position can also be differentiated allowing to apply a velocity dependent external force. A velocity dependent feedback control (VFC) has been recently implemented to reduce thermal noise of a cantilever in atomic force microscopy (AFM) [26] and in dynamic force microscopy [44]. A contribution to a rigorous thermodynamical foundation of macromolecules under (VFC) operating in nonequilibrium steady state is provided in [21]. The entropy production rate is there decomposed into a *positive entropy production rate* (PEPR) and an *entropy pumping rate* (EPuR). The latter indicates how much entropy is pumped out or into the macromolecule by the control force. It may render the overall entropy production negative. This is at the basis of a macromolecular cooling mechanism [6, 26, 44].

In this paper, we study entropy production in the presence of an external force in a more general situation. Our approach is new and complementary to [21] in that we study the free energy change rather than the total entropy change of the heat bath and of the Brownian particles as done in [21]. As “distance” between two probability densities associated to the unperturbed and perturbed evolution we employ the information *relative entropy* (in the quantum case, the von Neumann relative entropy for density operators). We show that it is possible to derive some basic formulas on the entropy production rate that extend those of [21] whenever the evolution of the physical system is in some suitable sense *Markovian*. We study nonequilibrium thermodynamical systems with finitely many degrees of freedom. Corresponding results are also sketched for  $n$ -level closed and open quantum systems. The perturbation of the Hamiltonian is interpreted as a *control function* which is designed by the controller in order to obtain a desired behavior of the system (reduction of thermal

noise, transfer to another state, etc.). Among potential applications, we mention molecular kinetics [11], macromolecular cooling [6, 21, 26, 44], quantum computation [34]. As it is well-known, relative entropy plays a central role in many areas of modern science besides physics such as mathematical statistics, information theory, probability, signal processing and quantum information processing, see e.g. [4, 7, 9, 10, 14, 15, 16, 22, 23, 37, 38, 40, 46] and references therein. Some of these results have been announced without proofs in our conference papers [35, 36].

The paper is outlined as follows. In the next section, we consider finite dimensional, nonequilibrium thermodynamical systems. In Section III, we derive a basic formula on relative entropy evolution for probability densities satisfying a continuity type equation. This result is then applied in the following section to controlled thermodynamic systems. Section V is devoted to the study of von Neumann entropy production for closed and open finite-dimensional quantum systems. In the Appendix, we show that the basic result may also be extended to *non-Markovian* finite-energy diffusions.

## II. THERMODYNAMIC SYSTEMS

Consider an open thermodynamic system whose macroscopic evolution is modelled by an  $n$ -dimensional Markov diffusion process  $\{x(t); t_0 \leq t\}$ . The components of  $x$  form a *complete set*, i.e. all other variables have a much shorter relaxation time [17]. Let  $\bar{\rho}(x)$  be the Maxwell-Boltzmann probability density corresponding to thermodynamical equilibrium

$$\bar{\rho}(x) = Z^{-1} \exp\left[-\frac{H(x)}{kT}\right]. \quad (\text{II.1})$$

Here  $H$  is the (continuously differentiable) Hamiltonian function, and the (forward) Ito differential of  $x$  is

$$dx(t) = \left[ -\frac{1}{2kT} \Sigma \Sigma^T \nabla H(x(t)) + u(x(t), t) \right] dt + \Sigma dW, \quad (\text{II.2})$$

where  $W$  is a standard  $n$ -dimensional Wiener process. The probability density  $\rho_t$  of  $x(t)$  satisfies the *Fokker-Planck equation*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left[ \left( -\frac{1}{2kT} \Sigma \Sigma^T \nabla H + u \right) \rho \right] = \frac{1}{2} \sum_{i,j=1}^n (\Sigma \Sigma^T)_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j}. \quad (\text{II.3})$$

In the uncontrolled case  $u = 0$ , under reasonable assumptions, see e.g. [25], as  $t \rightarrow \infty$ , the density  $\rho_t$  of  $x(t)$  tends to  $\bar{\rho}$  in *relative entropy* and, consequently, in total variation [24]. For the ergodic properties of this class of diffusions see e.g. [43, Section 7.5].

**Example II.1** In polymer dynamics [12], the *macromolecule* is described by a Hamiltonian

$$H(x, y) = \frac{1}{2} \langle y, My \rangle + \varphi(x),$$

where  $M$  stands for the direct sum

$$M = M_1 \oplus \cdots \oplus M_N, \quad M_k = m_k I_3, \quad k = 1, \dots, N,$$

Here  $x$  and  $y$  are  $3N$ -dimensional vectors, with  $x_i, y_i$  3-dimensional position and momentum of  $i$ th hard building block of macromolecule. Moreover,  $\varphi(x)$  is the *internal potential* of macromolecule (in AFM experiment [26],  $\varphi(x) = Kx^2/2$ , where  $K$  is the spring constant of cantilever). Random collisions between solvent water molecules and building blocks of macromolecule are modeled by the formal derivative of a Wiener process, namely *Gaussian white noise*. The six dimensional stochastic process  $(q_{i,x}, q_{i,y}, q_{i,z}, p_{i,x}, p_{i,y}, p_{i,z})$  associated the  $i$ th block obeys the equation

$$dq_{i\alpha} = \partial_{p_{i\alpha}} H(q, p) dt, \quad (\text{II.4})$$

$$dp_{i\alpha} = [-\partial_{q_{i\alpha}} H(q, p) + f_{i\alpha} + u_{i\alpha}(q, p)] dt + \Gamma_{i\alpha}^{j\beta} dW_{j\beta}(t), \quad (\text{II.5})$$

where Einstein's convention has been used. Here  $f$  is a frictional force,  $u$  a *position-velocity dependent control*. In the AFM experiment,  $f = -\gamma V$ ,  $u = -\alpha V$ ,  $\gamma > 0$ ,  $\alpha > 0$ , with  $V$  a velocity. The control here acts *like* a frictional force on the macromolecule. Since the frictional coefficient has been increased, one can introduce an *effective* temperature  $T_{\text{eff}}$  which is lower than the thermostat temperature  $T$ . As is well-known, different uncontrolled ( $u = 0$ ) versions of this model [19] play an important role also in other applications such as nonlinear circuits with noisy resistors [45].

To simplify the writing, we shall assume henceforth that in (II.2)  $\Sigma\Sigma^T = \sigma^2 I_n$ . The results of this paper, however, extend in a straightforward way to the case where the diffusion matrix  $\Sigma\Sigma^T$  is any symmetric, non negative definite (possibly singular as in (II.4)-(II.5)) matrix. Let us first recall a few basic concepts concerning the uncontrolled, nonequilibrium system (II.2). Let us introduce the *fluxes*  $J(x, t)$  and *forces*  $\Phi(x, t)$  by

$$\begin{aligned} J(x, t) &= -\frac{1}{2}\sigma^2\nabla\rho_t(x) - \frac{1}{2kT}\sigma^2\nabla H(x)\rho_t(x) \\ \Phi(x, t) &= -\nabla\mu(x, t), \end{aligned}$$

where  $\mu = H + kT \log \rho_t$  is the *electrochemical potential*. Notice the following:

1. The Fokker-Plank equation (II.3) may be rewritten (see e.g. [17]) as a continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla \cdot J = 0. \quad (\text{II.6})$$

2. Both fluxes and forces are zero in equilibrium. Moreover,

$$J(x, t) = \frac{\sigma^2}{2kT}\Phi(x, t)\rho_t(x), \quad (\text{II.7})$$

which plays the role of *constitutive relations*.

3. For  $\rho$  and  $\sigma$  nonnegative measurable functions on  $\mathbb{R}^n$ , we define the information *relative entropy* (*divergence*, *Kullback-Leibler distance*) by

$$\mathbb{D}(\rho||\sigma) = \int_{\mathbb{R}^n} \log \frac{\rho}{\sigma} \rho \, dx.$$

As it is well known [22], when  $\rho$  and  $\sigma$  are integrable functions with

$$\int_{\mathbb{R}^n} \rho(x) dx = \int_{\mathbb{R}^n} \sigma(x) dx,$$

we have  $\mathbb{D}(\rho||\sigma) \geq 0$ . Moreover,  $\mathbb{D}(\rho||\sigma) = 0$  if and only if  $\rho = \sigma$ . Define the *free energy* functional

$$F(\rho_t) = kT \int_{\mathbb{R}^n} \log \frac{\rho_t}{\bar{\rho}} \rho_t \, dx = kT \mathbb{D}(\rho_t||\bar{\rho}).$$

The free energy decay may now be expressed as [17]

$$\frac{d}{dt}F(\rho_t) = -\frac{\sigma^2 kT}{2} \int_{\mathbb{R}^n} |\nabla \log \frac{\rho_t}{\bar{\rho}}|^2 \rho_t \, dx = - \int J(x, t) \Phi(x, t) dx. \quad (\text{II.8})$$

Suppose now that, like in the AFM experiment, the thermodynamic system is subject to a feedback control action so that the macroscopic evolution is given by (II.2) with  $u \neq 0$ . The density  $\rho_t^u$  of the solution  $x_t^u$  satisfies the controlled Fokker-Planck equation (II.3). We are interested in the evolution of  $\mathbb{D}(\rho_t^u || \rho_t^0)$ , where  $\{\rho_t^0, t \geq t_0\}$  is an uncontrolled evolution ( $u \equiv 0$ ) . We first need a simple but useful result.

### III. A RELATIVE ENTROPY PRODUCTION FORMULA

Consider two families of nonnegative functions on  $\mathbb{R}^n$  :  $\{\rho_t; t_0 \leq t \leq t_1\}$  and  $\{\tilde{\rho}_t; t_0 \leq t \leq t_1\}$ . We are interested in how the relative entropy  $\mathbb{D}(\tilde{\rho}_t || \rho_t)$  evolves in time.

**Assumptions:**

- **A1** There exist measurable functions  $f(x, t)$  and  $\tilde{f}(x, t)$  such that  $\{\rho_t; t_0 \leq t \leq t_1\}$  and  $\{\tilde{\rho}_t; t_0 \leq t \leq t_1\}$  are everywhere positive  $C^1$  solutions of

$$\frac{\partial \rho_t}{\partial t} + \nabla \cdot (f \rho_t) = 0, \quad (\text{III.9})$$

$$\frac{\partial \tilde{\rho}_t}{\partial t} + \nabla \cdot (\tilde{f} \tilde{\rho}_t) = 0. \quad (\text{III.10})$$

- **A2**

For every  $t \in [t_0, t_1]$

$$\begin{aligned} \lim_{|x| \rightarrow \infty} f(x, t) \tilde{\rho}_t(x) &= 0, \\ \lim_{|x| \rightarrow \infty} \tilde{f}(x, t) \tilde{\rho}_t(x) &= 0, \\ \lim_{|x| \rightarrow \infty} \tilde{f}(x, t) \tilde{\rho}_t(x) \log \frac{\tilde{\rho}_t}{\rho_t}(x) &= 0. \end{aligned}$$

**Theorem III.1** Suppose  $\mathbb{D}(\tilde{\rho}_t || \rho_t) < \infty, \forall t \geq 0$ . Assume moreover A1 and A2 above. Then

$$\frac{d}{dt} \mathbb{D}(\tilde{\rho}_t || \rho_t) = \int_{\mathbb{R}^n} \left[ \nabla \log \frac{\tilde{\rho}_t}{\rho_t} \cdot (\tilde{f} - f) \right] \tilde{\rho}_t dx.$$

**Proof.**

$$\begin{aligned} \frac{d}{dt} \mathbb{D}(\tilde{\rho}_t || \rho_t) &= \int_{\mathbb{R}^n} \frac{d}{dt} [(\log \tilde{\rho}_t - \log \rho_t) \tilde{\rho}_t] dx \\ &= \int_{\mathbb{R}^n} \left\{ \left[ \frac{1}{\tilde{\rho}_t} \frac{\partial \tilde{\rho}_t}{\partial t} - \frac{1}{\rho_t} \frac{\partial \rho_t}{\partial t} \right] \tilde{\rho}_t + \log \frac{\tilde{\rho}_t}{\rho_t} \frac{\partial \tilde{\rho}_t}{\partial t} \right\} dx \\ &= \int_{\mathbb{R}^n} \left[ -\nabla \cdot (\tilde{f} \tilde{\rho}_t) + \frac{\tilde{\rho}_t}{\rho_t} \nabla \cdot (f \rho_t) - \log \frac{\tilde{\rho}_t}{\rho_t} \nabla \cdot (\tilde{f} \tilde{\rho}_t) \right] dx \\ &= \int_{\mathbb{R}^n} \left[ \nabla \log \frac{\tilde{\rho}_t}{\rho_t} \cdot \tilde{f} \tilde{\rho}_t - \nabla \frac{\tilde{\rho}_t}{\rho_t} \cdot f \frac{\rho_t}{\tilde{\rho}_t} \tilde{\rho}_t \right] dx = \int_{\mathbb{R}^n} \left[ \nabla \log \frac{\tilde{\rho}_t}{\rho_t} \cdot (\tilde{f} - f) \right] \tilde{\rho}_t dx, \end{aligned}$$

where we have used (III.9)-(III.10) and integration by parts (the boundary terms are zero because of Assumption 2). Q.E.D.

For  $\rho_t(x) \equiv 1$ , we have that  $-\mathbb{D}(\tilde{\rho}_t || \rho_t) = S(\tilde{\rho}_t)$  the entropy. Taking  $f(x, t) \equiv 0$ , we see that the first condition in A2 is verified. Theorem III.1 then gives (exchanging  $\rho_t$  with  $\tilde{\rho}_t$ ):

**Corollary III.2** Suppose  $\{\rho_t; t_0 \leq t \leq t_1\}$  is of class  $C^1$  and

$$\lim_{|x| \rightarrow \infty} v(x, t) \rho_t(x) = 0, \quad \lim_{|x| \rightarrow \infty} v(x, t) \rho_t(x) \log \rho_t(x) = 0.$$

Suppose  $S(\rho_t) < \infty, \forall t \in [t_0, t_1]$ . Then

$$\frac{d}{dt} S(\rho_t) = - \int_{\mathbb{R}^n} [\nabla \log \rho_t \cdot f] \rho_t dx. \quad (\text{III.11})$$

#### IV. ENTROPY PRODUCTION FOR CONTROLLED EVOLUTION

Consider now again the controlled thermodynamic system of Section II (II.2). Let  $\rho_t^u$  denote the density of the controlled process satisfying (II.3). We are interested in the evolution of  $\mathbb{D}(\rho_t^u || \rho_t^0)$ , where  $\{\rho_t^0, t \geq t_0\}$  is an uncontrolled evolution ( $u \equiv 0$ ). First of all, recall that the Fokker-Planck equations of the uncontrolled and controlled system may be written as continuity equations as in (II.6) Thus, we can apply Theorem III.1 with

$$f = -\frac{\sigma^2}{2kT} \nabla H(x) - \frac{\sigma^2}{2} \nabla \log \rho_t^0(x), \quad \tilde{f} = -\frac{\sigma^2}{2kT} \nabla H(x) + u(x, t) - \frac{\sigma^2}{2} \nabla \log \rho_t^u(x).$$

We get

$$\frac{d}{dt} \mathbb{D}(\rho_t^u || \rho_t^0) = \int_{\mathbb{R}^n} \left( \nabla \log \frac{\rho_t^u}{\rho_t^0} \cdot \left( u - \frac{\sigma^2}{2} \nabla \log \frac{\rho_t^u}{\rho_t^0} \right) \right) \rho_t^u dx. \quad (\text{IV.12})$$

Suppose now  $\rho_t^0 \equiv \bar{\rho}$ , where  $\bar{\rho}$  is the Maxwell-Boltzmann distribution (II.1). We get

**Theorem IV.1** Under assumptions A1 and A2,

$$\frac{d}{dt} \mathbb{D}(\rho_t^u || \bar{\rho}) = -\frac{\sigma^2}{2} \int_{\mathbb{R}^n} \left\| \nabla \log \frac{\rho_t^u}{\bar{\rho}} \right\|^2 \rho_t^u dx + \int_{\mathbb{R}^n} \nabla \log \frac{\rho_t^u}{\bar{\rho}} \cdot u \rho_t^u dx. \quad (\text{IV.13})$$

**Remark IV.2** Formula (IV.13) generalizes the decomposition of the entropy production exhibited in [21] for the controlled Langevin equations. In [21], the total entropy change of the heat bath and of the Brownian macromolecules is studied. The entropy production rate (EPR) is decomposed into the sum of two terms. The first, named PEPR (*positive entropy production rate*), is an always positive term expressed as the product of the thermodynamic force and the corresponding flux as in (II.8). The second, named EPuR (*entropy pumping rate*), describes the amount of entropy pumped out of or into the macromolecule by the



external agent. We recognize that (IV.13) implies that  $-\frac{d}{dt}\mathbb{D}(\rho_t^u||\bar{\rho})$  is also decomposed into an always positive term and into a term depending explicitly on the control function.

One can try to employ (IV.13) to analyze macromolecular cooling [6, 21, 26, 44]. Another direction of application is the following. Suppose we are interesting in modifying the rate at which the solution  $\rho_t$  of (II.3) tends to the invariant density (II.1). Let

$$\alpha(t) > -\frac{\sigma^2}{2},$$

and consider in (II.2) the feedback control

$$u(x, t) = -\alpha(t)\nabla \log \frac{\rho_t^u}{\bar{\rho}}(x). \quad (\text{IV.14})$$

Then,  $\rho_t^u$  satisfies the Fokker-Planck equation

$$\frac{\partial \rho^u}{\partial t} - \nabla \cdot \left( \left( \frac{\sigma^2}{2} + \alpha(t) \right) \frac{1}{kT} \nabla H \rho^u \right) = \left( \frac{\sigma^2}{2} + \alpha(t) \right) \Delta \rho^u. \quad (\text{IV.15})$$

A few observations are now in order.

1. Although the feedback control law is *nonlinear* in  $\rho_t^u$ , equation (IV.15) is *linear*;
2. the initial value problem for equation (IV.15) is well posed since  $\frac{\sigma^2}{2} + \alpha(t) > 0$ ;
3. equation (IV.15) still has as invariant density the Maxwell-Boltzmann distribution (II.1);
4. it is conceivable to solve (IV.15) off-line, and consequently compute the feedback law (IV.14) beforehand.
5. the flow of one dimensional probability densities  $\{\rho_t^u; t \geq 0\}$  of  $x^u(t)$  satisfying (II.2) with the control given by (IV.14) is the same as for the uncontrolled stochastic process  $\xi$  with differential

$$d\xi = - \left( \frac{\sigma^2}{2} + \alpha(t) \right) \frac{1}{kT} \nabla H(\xi) dt + \sqrt{\sigma^2 + 2\alpha(t)} dW, \quad (\text{IV.16})$$

provided  $\xi(0)$  is distributed according to  $\rho_0^u$ .

6. the friction and diffusion coefficients in (IV.16), although time-varying, still satisfy Einstein fluctuation-dissipation relation, see e.g [31].

We now employ (IV.13) to compute the relative entropy derivative. We get

$$\frac{d}{dt}\mathbb{D}(\rho_t^u||\bar{\rho}) = -\left(\frac{\sigma^2}{2} + \alpha(t)\right) \int_{\mathbb{R}^n} |\nabla \log \frac{\rho_t^u}{\bar{\rho}}|^2 \rho_t^u dx. \quad (\text{IV.17})$$

Hence, the controlled diffusion still tends to the Maxwell-Boltzmann distribution but at a different, “modulated” rate. In the linear Gauss-Markov case (i.e. when  $H$  is quadratic), the results assume a very concrete form. In particular, equation (IV.15) may be replaced by a linear matricial equation, see [36] for details.

The results of this section may be readily extended to non-Markovian, finite-energy diffusions employing the Nelson-Föllmer kinematics [13, 32], see the Appendix. Notice that this family plays a central role in several branches of mathematical physics, see e.g. [14, 33]. The results also extend without too much difficulty to a large class of diffusions with constant but singular diffusion coefficient such as in the case of the Orstein-Uhlenbeck model of physical Brownian motion [31] or, more generally, in the case of model (II.4)-(II.5). They may also be established for a large class of Markovian diffusion processes with local diffusion coefficient given the results in [18, 28, 29, 30, 31].

## V. $n$ -LEVEL QUANTUM SYSTEMS

It is apparent that Theorem III.1 can be applied to statistical mixtures in classical mechanics [35, Section IV]. Indeed, Liouville’s equation, expressing conservation of density in phase space, is just a continuity equation for the Hamiltonian evolution. One then gets the idea that it might be possible to establish a similar result in the quantum case, replacing the Liouville equation with the Landau-von Neumann equation for the density operator. First of all, we need to recall the basic formalism of statistical quantum mechanics.

### A. Closed quantum systems

As in standard quantum mechanics [39], to every physical system  $S$  is associated a complex Hilbert space  $\mathcal{H}_S$ . In the standard formulation, the state of the system is described by a unit vector  $\psi \in \mathcal{H}_S$ . For the sake of simplicity, here we will consider only finite dimensional Hilbert spaces, but results hold in the general case.

We consider situations in which uncertainty on the system state affects our model. The quantum analogue of a classical probability density is a density operators  $\rho$  in  $\mathcal{H}_S$ : A density operator is a positive semi-definite, unit trace operator on  $\mathcal{H}_S$ . They form a convex set  $\mathcal{D}(\mathcal{H}_S)$  and the extremals of  $\mathcal{D}(\mathcal{H}_S)$  are the one dimensional orthogonal projections. These are called *pure states*, and are equivalent to unit vectors in  $\mathcal{H}_S$  up to an overall phase factor, by setting  $\rho = \langle \psi, \cdot \rangle \psi$ . Physical observables are represented by Hermitian operators on  $\mathcal{H}_S$ .

Let  $A$  be an observable: The expected value of  $A$  for a system described by a density operator  $\rho$  is defined as:

$$\langle a \rangle_\rho := \text{trace}(\rho A). \quad (\text{V.18})$$

Hence, the variance for an observable  $A$  given  $\rho$  is naturally defined as

$$\text{Var}(A)_\rho := \langle (A - \langle a \rangle_\rho)^2 \rangle_\rho. \quad (\text{V.19})$$

It is easy to see that if  $\rho_p$  is a pure state, then exists an observable  $A$  such that the variance  $\text{Var}(A)_{\rho_p} = 0$ , clarifying the definition and the analogy with the classical case. The time evolution for the density operator of an isolated quantum system is determined by the Hamiltonian, i.e. the energy observable. The dynamical equation is the *Landau- von Neumann equation*:

$$i\hbar \frac{d}{dt} \rho_t = [H, \rho_t], \quad (\text{V.20})$$

where  $[\cdot, \cdot]$  denotes the commutator

$$[A, B] := AB - BA,$$

and  $\hbar$  is Planck's constant divided by  $2\pi$ .

Quantum analogues of entropic functionals have been considered since the very beginning of the mathematical foundation of quantum mechanics [47]. Recently renewed interest came from Quantum Information applications [34]. We are interested here in the quantum relative entropy, that is defined as:

$$\mathbb{D}(\rho||\tilde{\rho}) := \text{trace } (\rho(\log \rho - \log \tilde{\rho})). \quad (\text{V.21})$$

We define  $0 \log 0 = 0$ . As in the classical case, quantum relative entropy has the property of a pseudo-distance (see e.g. [34, 40]). We now consider the effect of a perturbation  $\Delta H$  on the evolution of quantum system originally driven by a free Hamiltonian  $H$  (we denote by  $\tilde{H} = H + \Delta H$  the perturbed Hamiltonian) .

**Proposition V.1** *Let  $\rho_t$  and  $\tilde{\rho}_t$  be the solution of (V.20) corresponding to the unperturbed and the perturbed Hamiltonians, respectively. The relative entropy production for the perturbed evolution is given by:*

$$\frac{d}{dt}\mathbb{D}(\rho||\tilde{\rho}) = \frac{i}{\hbar} < [\Delta H, \log \tilde{\rho}] >_{\rho} . \quad (\text{V.22})$$

**Proof.** Observing that  $[\rho, \log \rho] = 0$  and, consequently,

$$\frac{d}{dt}\text{trace } (\rho \log \rho) = 0,$$

(i.e. the *von Neumann entropy* is time invariant under Hamiltonian evolution), and using the cyclic property of trace, we have:

$$\begin{aligned} \frac{d}{dt}\mathbb{D}(\rho||\tilde{\rho}) &= \frac{d}{dt}\text{trace } (\rho \log \rho) + \frac{i}{\hbar}\text{trace } ([H, \rho] \log \tilde{\rho} + \rho[\tilde{H}, \log \tilde{\rho}]) \\ &= \frac{i}{\hbar}\text{trace } ([H, \rho \log \tilde{\rho}] + \rho[\Delta H, \log \tilde{\rho}]) \\ &= \frac{i}{\hbar}\text{trace } (\rho[\Delta H, \log \tilde{\rho}]) . \end{aligned} \quad (\text{V.23})$$

Q.E.D.

We remark that the initial conditions for the perturbed and the unperturbed evolution can be different, and we can easily exchange the role of perturbed and unperturbed evolution

adding a minus sign on the right hand side. The analogy with the corresponding relative entropy evolution formula in classical mechanics [35] is apparent. As in the classical case, the perturbation can be interpreted as an additive control Hamiltonian.

## B. Open Quantum Systems

When we consider a quantum system interacting with the environment in some uncontrollable way, namely an *open quantum system* [2, 34], the situation changes significantly. The complete dynamical description of the situation should be done considering the tensor product space of both the system and the environment space. Usually, the environment has too many degrees of freedom to be modelled. Moreover, only partial information about environment initial state interactions may be available. In these cases, we can still obtain a dynamical equation for the system state by averaging over the environment degrees of freedom [2]. If the system evolution is assumed to be Markovian, strongly continuous in time and completely positive [34], a general form for the generator of the system density operator dynamics is the following [27]:

$$\frac{d}{dt}\rho_t = -\frac{i}{\hbar}[H, \rho_t] + \mathcal{L}[\rho_t], \quad (\text{V.24})$$

where  $H$  is the effective Hamiltonian, in general different from the free drift Hamiltonian, and the generator for the dissipative evolution  $\mathcal{L}$  has the form:

$$\mathcal{L}[\rho] = \frac{1}{2} \sum_k \left( [L_k \rho, L_k^\dagger] + [L_k, \rho L_k^\dagger] \right). \quad (\text{V.25})$$

The operators  $L_k$  can be derived under different assumptions on the couplings with the environment or on a phenomenological basis (see e.g. [2] and reference therein). This equation can be seen as a quantum analogue of a Fokker-Planck equation, since it describes the time evolution of the density operator in the absence of conditioning measurements. Assume that (V.24) admits a stationary state commuting with the effective Hamiltonian,

and denote it with  $\bar{\rho}$ . Noting that:

$$\text{trace} \left( \rho \frac{d}{dt} \log \rho \right) = \text{trace} \left( \frac{d}{dt} \rho \right) = 0,$$

since the generator (V.24) has zero trace, we obtain for the relative entropy production (see also [42]):

$$\frac{d}{dt} \mathbb{D}(\rho || \bar{\rho}) = \text{trace} (\mathcal{L}[\rho](\log \rho - \log \bar{\rho})) \leq 0. \quad (\text{V.26})$$

The fact that  $\mathbb{D}(\rho || \bar{\rho})$  is non-increasing for the dynamical semigroup generated by (V.24) was established by Lindblad, see e.g. [2]. To extend this result to the case of a perturbed Hamiltonian, we consider now  $\bar{\rho}$  as a *fixed target state*, since the introduction of perturbations could in general change the stationary states. In this setting, we get:

$$\begin{aligned} \frac{d}{dt} \mathbb{D}(\rho || \bar{\rho}) &= \text{trace} \left( \frac{i}{\hbar} [\tilde{H}, \rho] \log \bar{\rho} + \mathcal{L}[\rho](\log \rho - \log \bar{\rho}) \right) \\ &= -\frac{i}{\hbar} \langle [\Delta H, \log \bar{\rho}] \rangle_{\rho} + \text{trace} (\mathcal{L}[\rho](\log \rho - \log \bar{\rho})), \end{aligned} \quad (\text{V.27})$$

where now  $\rho$  is undergoing a *perturbed evolution*  $\tilde{H} = H + \Delta H$  and  $[\bar{\rho}, H] = 0$  as before. In the quantum case, however, the effectiveness of a control Hamiltonian is severely limited. For instance, in the closed system case, the density operator eigenvalues cannot be modified by a control Hamiltonian, precluding convergence in relative entropy if the target state has a different spectrum from the initial condition. A detailed analysis of the dissipative case from a control theoretic viewpoint can be found e.g. in [3, 41]. Whether these formulas could be of help in designing or analyzing control strategies will be a matter of further work (see also comments on this issue in [36, Section VII]).

Further analogies with the classical thermodynamics setting can be unravelled if we restrict our attention to equation (V.24) when it is derived from e.g. a *weak coupling* limit [2]. This is essentially a constructive derivation of equations of the form (V.24) from the joint (tensor) description of the system and the environment, that is consistent with classical thermodynamics. In fact, the Gibbs state:

$$\rho_G = Z^{-1} e^{-\beta H},$$

where  $Z$  is the *partition function* and  $H$  the system Hamiltonian, is a stationary state for the resulting equation. Since, as we already recalled, relative entropy with respect to the stationary state is non-increasing, for this class of dissipative Markovian evolutions we have a full correspondence with the classical mechanical case [35].

## VI. CONCLUSION AND OUTLOOK

We have derived explicit dependence of the *relative entropy production rate* on the control action for various uncertain physical systems exhibiting a *Markovian evolution*. Further work is needed to find other significant applications of the results as well as possible extension to other, more complex, systems with Markovian evolution such as interacting particle systems.

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## APPENDIX: FINITE-ENERGY DIFFUSIONS

Let  $\Omega := \mathcal{C}([t_0, t_1], \mathbb{R}^n)$  denote the family of  $n$ -dimensional continuous functions, and let  $P$  and  $\tilde{P}$  be two probability distributions on  $\Omega$ . The *relative entropy*  $H(\tilde{P}, P)$  of  $\tilde{P}$  with

respect to  $P$  is defined by

$$H(\tilde{P}, P) = \begin{cases} E_{\tilde{P}}[\log \frac{d\tilde{P}}{dP}] & \text{if } \tilde{P} \ll P \\ +\infty & \text{otherwise} \end{cases}$$

Let  $W_x$  denote Wiener measure on  $\Omega$  starting at  $x \in \mathbb{R}^n$ , and let

$$W := \int W_x dx$$

be stationary Wiener measure. Let  $\sigma > 0$ , and denote by  $\mathbb{D}$  be the family of distributions  $P$  on  $\Omega$  such that  $H(P, \sigma W) < \infty$ . Let  $\mathcal{F}_t$  and  $\mathcal{G}_t$  denote the  $\sigma$ -algebras of events observable up to time  $t$  and from time  $t$  on, respectively. It then follows from the Girsanov's theory [13, 20] that  $P \in \mathbb{D}$  possesses both a forward drift  $\beta^P$  and a backward drift  $\gamma^P$ , namely under  $P$ , the increments of the canonical coordinate process  $x(t, \omega) = \omega(t)$  admit the representations

$$x(t) - x(s) = \int_s^t \beta^P(\tau) d\tau + \sigma[w_+(t) - w_+(s)], \quad t_0 \leq s < t \leq t_1, \quad (.1)$$

$$x(t) - x(s) = \int_s^t \gamma^P(\tau) d\tau + \sigma[w_-(t) - w_-(s)], \quad t_0 \leq s < t \leq t_1. \quad (.2)$$

$\beta^P(t)$  is at each time  $t$   $\mathcal{F}_t$ -measurable and  $w_+(\cdot)$  is a standard,  $n$ -dimensional Wiener process. Symmetrically,  $\gamma^P(t)$  is  $\mathcal{G}_t$ -measurable and  $w_-$  is another standard Wiener process. Moreover,  $\beta^P$  and  $\gamma^P$  satisfy the finite-energy condition

$$E \left\{ \int_{t_0}^{t_1} \beta^P(t) \cdot \beta^P(t) dt \right\} < \infty, \quad E \left\{ \int_{t_0}^{t_1} \gamma^P(t) \cdot \gamma^P(t) dt \right\} < \infty. \quad (.3)$$

It was shown in [13] that the one-time probability density  $p_t(\cdot)$  of  $x(t)$  (which exists for every  $t$ ) is absolutely continuous on  $\mathbb{R}^n$  and the following relation holds a.s.  $\forall t > 0$

$$E\{\beta^P(t) - \gamma^P(t) | x(t)\} = \sigma^2 \nabla \log p_t(x(t)). \quad (.4)$$

Let us introduce the *current drift* and the *current drift field* of  $P$

$$v^P(t) = \frac{\beta^P(t) + \gamma^P(t)}{2}, \quad v^P(x, t) = E\{v^P(t) | x(t) = x\}. \quad (.5)$$

Then, the one-time density  $p_t$  satisfies weakly [32] a continuity type equation

$$\frac{\partial p_t}{\partial t} + \nabla \cdot (v^P p_t) = 0. \quad (.6)$$

Hence, Theorem III.1 holds true for finite energy diffusions provided we define the  $v$  fields according to (.5).